Glycine, N,N-dimethyl-1118-68-9 | DTXSID6074336

Model Performance

Marada I	D. L.
Model	Data
110001	Bata

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 40.1 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.30e-01

Confidence level: 7.35e-01

Nearest Neighbors from the Training Set

Image not found

Diethylacetamide Measured: 69.2 Predicted: 64.5 Image not found

Daminozide Measured: 8.91 Predicted: 10.9 Image not found

Benzamide, N,N-dimethyl-

Measured: 39.8 Predicted: 36.3

Image not found

Allidochlor Measured: 20.0 Predicted: 24.7 Image not found

N,N-Dimethylaniline Measured: 182 Predicted: 130